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AN INTERCOMPARISON OF MEDIUM ENERGY CROSS-SECTION CODES

Sol Pearlstein

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Abstract

Five medium energy proton reaction cases are selected for benchmarking nuclear model codes. The quantities calculated are isotopic activation yields for 180 MeV protons on Al and 40-200 MeV protons on Co, and double differential neutron emission spectra from Al, Zr-90 and Pb-208 for 35, 80, 160, 318, and 800 MeV proton bombardment. The five codes for which results are presented consist of three types: (1) a closed form preequilibrium plus evaporation model, (2) an intranuclear-cascade and evaporation model, and (3) a model relying on nuclear systematics. The characteristics of each code are described. There are orders of magnitude differences in the time for each type of code to calculate neutron emission spectra, with codes using systematics, preequilibrium and intranuclear-cascade models requiring seconds, minutes and hours, respectively. Calculations are not compared with experiment in this initial study.

For double differential neutron emission spectra, there is good overall agreement in magnitude among the different types of codes at forward angles. Differences where they occur at forward angles are greatest for the mid-energy neutrons emitted. At back angles the incident energy at which the best overall agreement is obtained is 160 MeV and the material for which the best overall agreement is obtained is Al.

I. Benchmark Calculations

If ultimately the results of benchmark experiments of medium energy applications can be simulated using nuclear cross-section codes and radiation transport methods, engineering designs can be achieved relatively quickly and inexpensively with fewer experiments needed. Nuclear model code calculations can be compared to some nuclear cross-section measurements that are available but measurements of the same cross-section by different authors do not always converge to the same values. Similarly, different nuclear model codes do not always converge to the same value. It is helpful to understand what the cross-section codes themselves are doing. This report does not compare calculation with experiment. Instead, it compares the results from different codes calculating the same problem description. The calculational benchmarks chosen were of the type to anticipate experimental results that may be forthcoming.

It is hoped that this report will be part of a long range study to validate codes for medium energy applications. Extensions of this work will include comparisons with experimental data. Only partial results have been received to date but are considered sufficient to (1) provide information about the capability of codes, (2) compare the results obtained from different codes using similar input but different algorithms (or even ostensibly the same algorithms) for solution and (3) stimulate more contributions and additional benchmarks.

II. Benchmarks

The benchmark specifications for an intercomparison of cross-section codes were formulated at a May 1987 meeting of the Medium Energy Nuclear Data Working Group.¹ At that meeting a Codes and Models Subgroup chaired by M. Blann proposed the following five benchmarks:

Activation Yields

1. 180 MeV protons on Al-27
2. 40-200 MeV protons on Co-59

Neutron Emission Spectra

35, 80, 160, 318 and 800 MeV protons on

3. Al-27
4. Zr-90
5. Pb-208

The specifications for the 5 benchmark problems are given in Appendix I.

The benchmark problems were limited in scope so that the comparison of the results would not be too cumbersome, time consuming or error prone. Fortunately, most results were received in computerized form greatly reducing the labor involved and the chances for errors.

III. Code Results Submitted

The codes for which results were received consisted of two types of algorithm solutions, (1) deterministic, for which a given set of input produces a unique answer, and (2) Monte Carlo, for which a given set of input produces a statistically determined answer whose convergence improves as the number of trials is increased.

The cross section model codes for which results were received consisted of three types, (1) a closed form preequilibrium plus evaporation model, (2) an intranuclear-cascade and evaporation model, and (3) a model relying on nuclear systematics. An example of the first type of code is ALICE² which uses Weisskopf-Ewing evaporation, Bohr-Wheeler rotating drop fission competition and the exciton preequilibrium models to describe nuclear reactions. Examples of the second type of code are various versions of the high energy transport code HETC which are extensions of the Bertini³ model. Both ALICE and HETC attempt to physically model nuclear reactions and rely on very few empirically determined parameters. An example of the third type of code is PNEM which uses semiphysical evaporation shapes to fit experimental neutron emission spectra from proton induced reactions.⁴ These data are observed to vary nearly monotonically with increasing energy, mass, and angle. The PNEM parameters were empirically determined for the energy range

about 590 MeV, so that the agreement between calculation and experiment should be quite good, but that is not the subject of this first stage investigation. Unlike the other codes discussed here which calculate a wide variety of nuclear cross-sections, PNEM mainly calculates the double differential neutron emission cross-section.

The results from five codes are discussed in this report.

1. ALICE, submitted by Marshall Blann, Lawrence Livermore National Laboratory
2. ALICE-B, submitted by Sol Pearlstein, Brookhaven National Laboratory
3. HETC-F (TIERCE), submitted by Claude Philis, CEA, Bruyeres-le-Chatel
4. HETC-H (HETC-KFA-2), submitted by Detlef Filges, KFA, Juelich
5. PNEM, submitted by Sol Pearlstein, Brookhaven National Laboratory

Brief descriptions of each code were requested and are contained in Appendix II.

In a "blind" benchmark comparison the results would be published as received. In this initial study, a draft report was circulated to the submitters so that they could confirm that their data had been used correctly. An error was found in the HETC-H calculations and renormalized results were subsequently received and used for the comparison. An example of these changes is given in Section III.2.

III.1 Activation Yields

Tabulated results were received from M. Blann using ALICE and computation formatted results from S. Pearlstein using ALICE-B. Although results in computerized form had not been required it was soon evident that computerized results greatly facilitated the comparison. It was noted that the Blann and Pearlstein results differed because Blann had chosen the normal pairing shift ($MP=3$) and 3 output particles ($M3=3$) and Pearlstein had chosen the level density ground state shift with shell corrections included ($MP=2$) and 4 output particles ($M3=4$). For identical input the two codes produced identical results to 5 significant figures except for small differences where partial waves for impact angular momenta greater than 21 (a somewhat arbitrary present limit in ALICE but not in ALICE-B) were involved. On the one hand the exact agreement is not surprising because ALICE-B was derived from ALICE but on the other hand ALICE-B has several enhancements and has been adapted to run on a DEC-10 and VAX-780, with 36 and 32 bit words, respectively, whereas ALICE results are obtained on a CDC-7600, with 60 bit words.

Partial wave requirements for angular momenta greater than 21 are negligible for 180 MeV protons on Al-27 and protons below 140 MeV on Co-59. Therefore, the computation format output of ALICE-B which is essentially equivalent to those of ALICE, was used to facilitate the presentation of results. Also, since the differences between ALICE and ALICE-B calculations resulted from choices in input parameters rather than differences in the codes, it is useful to compare the effect of these input parameter choices, and others, on the results to illustrate their effect to present and potential users of the ALICE code.

For Benchmarks 1 and 2 the parameters used by Blann are shown in Table I.

Table I. ALICE Input Parameters for Benchmarks 1 and 2

NA = 11; The number of isotopes included for each residual element.
 NZ = 9; The number of elements included in the cascade calculations.
 MC = 10; Atomic masses option.
 MP = 3; Normal pairing shift option, 0 for odd-even nuclei, delta added to excitation for odd-odd nuclei.
 INVER = 2; Inverse cross-sections calculated by sharp cutoff method.
 M3 = 3; Neutrons, protons, and alphas emitted.

For Benchmark 1, 180 MeV protons on Al-27, the cross-section yields of activation products are shown in Figure 1 and listed in Table II.

For Benchmark 2, 40 to 200 MeV protons on Co-59, the cross-section yields of activation products at 20 MeV steps (received in 10 MeV steps) are listed in Table III. Graphical displays at 120, 160, and 200 MeV are shown in Figure 2.

For Benchmark 2, the ALICE options listed in Table IV were used for calculations. The activation cross-sections for Co-56, Mn-54, and V-50 using Table IV options are shown in Figure 3.

Table II. Yield Cross-Section of Activation Products from 180 MeV Protons on Al-27

YIELD CROSS-SECTION (MB)											
Z/A	28	27	26	25	24	23	22	21	20	19	18
14	0.000E+00	0.404E+01	0.182E+01	0.201E-01	0.340E-03	0.552E-04	0.297E-06	0.455E-08	0.000E+00	0.000E+00	0.000E+00
13	0.719E+01	0.185E+02	0.533E+01	0.312E+00	0.111E-01	0.545E-03	0.648E-05	0.422E-07	0.266E-11	0.154E-25	0.000E+00
12	0.870E+01	0.261E+02	0.379E+02	0.103E+02	0.469E+00	0.113E-01	0.333E-03	0.415E-05	0.421E-08	0.310E-11	0.000E+00
11	0.398E+00	0.273E+01	0.289E+02	0.321E+02	0.355E+01	0.197E+00	0.562E-02	0.409E-04	0.326E-06	0.801E-10	0.568E-18
10	0.135E-01	0.198E+00	0.245E+01	0.150E+02	0.134E+02	0.189E+01	0.595E-01	0.212E-02	0.000E+00	0.881E-07	0.000E+00
9	0.100E-02	0.773E-02	0.929E-01	0.867E+00	0.357E+01	0.592E+01	0.775E+00	0.362E-01	0.380E-03	0.232E-05	0.306E-08
8	0.798E-05	0.125E-03	0.260E-02	0.311E-01	0.197E+00	0.202E+01	0.182E+02	0.257E+01	0.139E-01	0.547E-04	0.000E+00
7	0.552E-07	0.353E-06	0.269E-04	0.283E-03	0.652E-02	0.143E+00	0.483E+01	0.655E+01	0.704E+00	0.223E-02	0.127E-04
6	0.120E-10	0.424E-10	0.718E-07	0.185E-05	0.311E-04	0.125E-02	0.416E-01	0.192E+01	0.506E+01	0.103E+00	0.304E-03

Table III. Yield Cross-Sections of Activation Products from Protons on Co-59

IIIa. 40 MeV Yield Cross-Section (MB)

YIELD CROSS-SECTION (MB)											
Z/A	60	59	58	57	56	55	54	53	52	51	50
28	0.000E+00	0.220E+02	0.442E+02	0.418E+02	0.220E+02	0.201E-01	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
27	0.421E+02	0.809E+02	0.132E+03	0.211E+03	0.352E+02	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
26	0.134E+02	0.202E+02	0.595E+02	0.547E+02	0.109E+02	0.139E+02	0.258E-01	0.000E+00	0.000E+00	0.000E+00	0.000E+00
25	0.138E+00	0.900E+00	0.145E+01	0.920E+01	0.386E+02	0.176E+01	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
24	0.213E-03	0.269E-04	0.143E+00	0.168E+01	0.367E+00	0.405E+00	0.994E+00	0.234E-04	0.000E+00	0.000E+00	0.000E+00
23	0.000E+00	0.000E+00	0.566E-03	0.500E-05	0.108E+00	0.277E+00	0.123E-03	0.000E+00	0.000E+00	0.000E+00	0.000E+00
22	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.125E-02	0.177E-07	0.566E-02	0.490E-02	0.000E+00	0.000E+00	0.000E+00
21	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.148E-04	0.000E+00	0.000E+00	0.000E+00	0.000E+00
20	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.124E-07	0.000E+00	0.000E+00

IIIb. 60 MeV Yield Cross-Section (MB)

YIELD CROSS-SECTION (MB)											
Z/A	60	59	58	57	56	55	54	53	52	51	50
28	0.000E+00	0.292E+02	0.851E+02	0.190E+03	0.693E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
27	0.530E+02	0.118E+03	0.348E+03	0.489E+01	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
26	0.130E+02	0.253E+02	0.226E+01	0.896E+01	0.472E+02	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
25	0.159E-01	0.000E+00	0.325E+01	0.122E+02	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
24	0.000E+00	0.000E+00	0.225E-01	0.000E+00	0.506E+00	0.460E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
23	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.713E-02	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
22	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.889E-06	0.000E+00	0.000E+00	0.000E+00	0.000E+00
21	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
20	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00

IIIc. 80 MeV Yield Cross-Section (MB)

YIELD CROSS-SECTION (MB)

Z\A	60	59	58	57	56	55	54	53	52	51	50
28	0.000E+00	0.165E+02	0.284E+02	0.224E+02	0.840E+01	0.376E+00	0.112E-02	0.000E+00	0.000E+00	0.000E+00	0.000E+00
	59	58	57	56	55	54	53	52	51	50	49
27	0.320E+02	0.659E+02	0.910E+02	0.112E+03	0.630E+02	0.313E+01	0.126E-03	0.000E+00	0.000E+00	0.000E+00	0.000E+00
	58	57	56	55	54	53	52	51	50	49	48
26	0.139E+02	0.183E+02	0.536E+02	0.757E+02	0.610E+02	0.527E+01	0.210E+01	0.200E-02	0.000E+00	0.000E+00	0.000E+00
	57	56	55	54	53	52	51	50	49	48	47
25	0.160E+00	0.130E+01	0.544E+01	0.969E+01	0.196E+02	0.262E+02	0.323E+01	0.170E-05	0.000E+00	0.000E+00	0.000E+00
	56	55	54	53	52	51	50	49	48	47	46
24	0.751E-03	0.143E-01	0.142E+00	0.147E+01	0.759E+01	0.322E+01	0.609E+00	0.934E+00	0.732E-02	0.000E+00	0.000E+00
	55	54	53	52	51	50	49	48	47	46	45
23	0.163E-05	0.450E-06	0.485E-02	0.792E-01	0.104E+00	0.474E+00	0.105E+01	0.909E-01	0.107E-07	0.000E+00	0.000E+00
	54	53	52	51	50	49	48	47	46	45	44
22	0.000E+00	0.000E+00	0.120E-04	0.785E-05	0.110E-01	0.678E-01	0.367E-01	0.972E-02	0.317E-01	0.498E-03	0.000E+00
	53	52	51	50	49	48	47	46	45	44	43
21	0.000E+00	0.000E+00	0.236E-16	0.000E+00	0.126E-03	0.799E-06	0.155E-02	0.345E-02	0.537E-04	0.000E+00	0.000E+00
	52	51	50	49	48	47	46	45	44	43	42
20	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.221E-12	0.000E+00	0.101E-04	0.127E-07	0.844E-04	0.145E-03	0.145E-06

IIId. 100 MeV Yield Cross-Section (MB)

YIELD CROSS-SECTION (MB)

Z\A	60	59	58	57	56	55	54	53	52	51	50
28	0.000E+00	0.151E+02	0.224E+02	0.154E+02	0.516E+01	0.241E+00	0.413E-02	0.218E-06	0.000E+00	0.000E+00	0.000E+00
	59	58	57	56	55	54	53	52	51	50	49
27	0.288E+02	0.553E+02	0.735E+02	0.757E+02	0.508E+02	0.722E+01	0.277E+00	0.291E-04	0.000E+00	0.000E+00	0.000E+00
	58	57	56	55	54	53	52	51	50	49	48
26	0.144E+02	0.150E+02	0.469E+02	0.767E+02	0.754E+02	0.184E+02	0.999E+00	0.513E-01	0.463E-04	0.000E+00	0.000E+00
	57	56	55	54	53	52	51	50	49	48	47
25	0.124E+00	0.151E+01	0.637E+01	0.149E+02	0.277E+02	0.183E+02	0.963E+01	0.422E+00	0.665E-05	0.000E+00	0.000E+00
	56	55	54	53	52	51	50	49	48	47	46
24	0.174E-02	0.177E-01	0.262E+00	0.164E+01	0.707E+01	0.109E+02	0.575E+01	0.519E+00	0.156E+00	0.106E-03	0.000E+00
	55	54	53	52	51	50	49	48	47	46	45
23	0.179E-04	0.233E-03	0.645E-02	0.105E+00	0.896E+00	0.809E+00	0.803E+00	0.131E+01	0.114E+00	0.401E-06	0.000E+00
	54	53	52	51	50	49	48	47	46	45	44
22	0.419E-08	0.387E-08	0.552E-04	0.203E-02	0.122E-01	0.912E-01	0.280E+00	0.158E+00	0.344E-01	0.255E-01	0.430E-03
	53	52	51	50	49	48	47	46	45	44	43
21	0.000E+00	0.000E+00	0.925E-07	0.175E-06	0.109E-02	0.505E-02	0.194E-02	0.132E-01	0.237E-01	0.841E-03	0.701E-08
	52	51	50	49	48	47	46	45	44	43	42
20	0.000E+00	0.000E+00	0.758E-17	0.000E+00	0.470E-05	0.113E-05	0.192E-03	0.915E-03	0.144E-03	0.286E-03	0.114E-02

Table IIIe. 120 MeV Yield Cross-Section (MB)

YIELD CROSS-SECTION (MB)											
Z/A	60	59	58	57	56	55	54	53	52	51	50
28	0.000E+00	0.118E+02	0.165E+02	0.120E+02	0.307E+01	0.170E+00	0.451E-02	0.421E-04	0.877E-08	0.000E+00	0.000E+00
	59	58	57	56	55	54	53	52	51	50	49
27	0.227E+02	0.452E+02	0.620E+02	0.609E+02	0.350E+02	0.621E+01	0.444E+00	0.639E-02	0.150E-06	0.000E+00	0.000E+00
	58	57	56	55	54	53	52	51	50	49	48
26	0.141E+02	0.139E+02	0.342E+02	0.715E+02	0.734E+02	0.245E+02	0.284E+01	0.540E-01	0.129E-02	0.196E-05	0.480E-13
	57	56	55	54	53	52	51	50	49	48	47
25	0.110E+00	0.117E+01	0.739E+01	0.151E+02	0.371E+02	0.314E+02	0.897E+01	0.217E+01	0.202E-01	0.182E-05	0.000E+00
	56	55	54	53	52	51	50	49	48	47	46
24	0.183E-02	0.304E-01	0.230E+00	0.191E+01	0.963E+01	0.108E+02	0.129E+02	0.383E+01	0.176E+00	0.604E-02	0.940E-05
	55	54	53	52	51	50	49	48	47	46	45
23	0.161E-04	0.424E-03	0.127E-01	0.150E+00	0.972E+00	0.292E+01	0.235E+01	0.144E+01	0.862E+00	0.417E-01	0.130E-05
	54	53	52	51	50	49	48	47	46	45	44
22	0.154E-06	0.167E-05	0.673E-04	0.330E-02	0.554E-01	0.160E+00	0.378E+00	0.986E+00	0.400E+00	0.346E-01	0.188E-01
	53	52	51	50	49	48	47	46	45	44	43
21	0.270E-10	0.124E-10	0.185E-05	0.621E-04	0.132E-02	0.149E-01	0.427E-01	0.241E-01	0.418E-01	0.579E-01	0.871E-02
	52	51	50	49	48	47	46	45	44	43	42
20	0.138E-24	0.000E+00	0.353E-09	0.544E-08	0.275E-04	0.291E-03	0.328E-03	0.276E-02	0.970E-02	0.389E-02	0.239E-02

Table IIIf. 140 MeV Yield Cross-Section (MB)

YIELD CROSS-SECTION (MB)											
Z/A	60	59	58	57	56	55	54	53	52	51	50
28	0.000E+00	0.935E+01	0.121E+02	0.948E+01	0.273E+01	0.111E+00	0.383E-02	0.731E-04	0.116E-05	0.321E-09	0.152E-19
	59	58	57	56	55	54	53	52	51	50	49
27	0.180E+02	0.391E+02	0.531E+02	0.488E+02	0.279E+02	0.577E+01	0.344E+00	0.204E-01	0.101E-03	0.143E-08	0.000E+00
	58	57	56	55	54	53	52	51	50	49	48
26	0.137E+02	0.140E+02	0.299E+02	0.508E+02	0.818E+02	0.220E+02	0.453E+01	0.140E+00	0.140E-02	0.534E-04	0.316E-07
	57	56	55	54	53	52	51	50	49	48	47
25	0.109E+00	0.991E+00	0.658E+01	0.179E+02	0.348E+02	0.340E+02	0.143E+02	0.197E+01	0.542E-01	0.659E-03	0.610E-07
	56	55	54	53	52	51	50	49	48	47	46
24	0.139E-02	0.312E-01	0.298E+00	0.163E+01	0.102E+02	0.154E+02	0.132E+02	0.872E+01	0.741E+00	0.985E-02	0.399E-03
	55	54	53	52	51	50	49	48	47	46	45
23	0.331E-04	0.378E-03	0.121E-01	0.206E+00	0.126E+01	0.285E+01	0.494E+01	0.442E+01	0.102E+01	0.301E+00	0.247E-02
	54	53	52	51	50	49	48	47	46	45	44
22	0.173E-06	0.377E-05	0.155E-03	0.323E-02	0.704E-01	0.388E+00	0.988E+00	0.866E+00	0.161E+01	0.465E+00	0.239E-01
	53	52	51	50	49	48	47	46	45	44	43
21	0.951E-09	0.857E-08	0.209E-05	0.148E-03	0.403E-02	0.152E-01	0.713E-01	0.160E+00	0.144E+00	0.102E+00	0.735E-01
	52	51	50	49	48	47	46	45	44	43	42
20	0.222E-13	0.250E-13	0.718E-08	0.399E-06	0.325E-04	0.730E-03	0.343E-02	0.491E-02	0.196E-01	0.430E-01	0.308E-01

IIIg. 160 MeV Yield Cross-Section (MB)

YIELD CROSS-SECTION (MB)

Z/A	60	59	58	57	56	55	54	53	52	51	50
28	0.000E+00	0.906E+01	0.100E+02	0.742E+01	0.222E+01	0.879E-01	0.256E-02	0.441E-04	0.169E-05	0.183E-07	0.475E-12
27	59	58	57	56	55	54	53	52	51	50	49
	0.171E+02	0.342E+02	0.469E+02	0.404E+02	0.235E+02	0.556E+01	0.484E+00	0.206E-01	0.422E-03	0.164E-05	0.476E-10
26	58	57	56	55	54	53	52	51	50	49	48
	0.128E+02	0.124E+02	0.296E+02	0.446E+02	0.696E+02	0.276E+02	0.326E+01	0.255E+00	0.481E-02	0.109E-03	0.509E-06
25	57	56	55	54	53	52	51	50	49	48	47
	0.958E-01	0.955E+00	0.578E+01	0.181E+02	0.367E+02	0.292E+02	0.163E+02	0.288E+01	0.563E-01	0.368E-02	0.153E-04
24	56	55	54	53	52	51	50	49	48	47	46
	0.154E-02	0.310E-01	0.375E+00	0.180E+01	0.915E+01	0.175E+02	0.200E+02	0.739E+01	0.155E+01	0.304E-01	0.664E-03
23	55	54	53	52	51	50	49	48	47	46	45
	0.478E-04	0.726E-03	0.107E-01	0.192E+00	0.176E+01	0.353E+01	0.463E+01	0.700E+01	0.229E+01	0.328E+00	0.853E-02
22	54	53	52	51	50	49	48	47	46	45	44
	0.116E-06	0.269E-05	0.190E-03	0.562E-02	0.678E-01	0.405E+00	0.119E+01	0.216E+01	0.199E+01	0.102E+01	0.133E+00
21	53	52	51	50	49	48	47	46	45	44	43
	0.277E-08	0.417E-07	0.235E-05	0.163E-03	0.679E-02	0.381E-01	0.940E-01	0.226E+00	0.460E+00	0.257E+00	0.927E-01
20	52	51	50	49	48	47	46	45	44	43	42
	0.159E-11	0.155E-10	0.110E-07	0.109E-05	0.106E-03	0.974E-03	0.681E-02	0.211E-01	0.388E-01	0.564E-01	0.127E+00

IIIh. 180 MeV Yield Cross-Section (MB)

YIELD CROSS-SECTION (MB)

Z/A	60	59	58	57	56	55	54	53	52	51	50
28	0.000E+00	0.744E+01	0.829E+01	0.632E+01	0.154E+01	0.702E-01	0.266E-02	0.558E-04	0.153E-05	0.780E-07	0.106E-09
27	59	58	57	56	55	54	53	52	51	50	49
	0.141E+02	0.293E+02	0.414E+02	0.373E+02	0.182E+02	0.460E+01	0.469E+00	0.187E-01	0.531E-03	0.774E-05	0.630E-08
26	58	57	56	55	54	53	52	51	50	49	48
	0.117E+02	0.116E+02	0.238E+02	0.413E+02	0.563E+02	0.294E+02	0.367E+01	0.239E+00	0.860E-02	0.174E-03	0.225E-05
25	57	56	55	54	53	52	51	50	49	48	47
	0.892E-01	0.809E+00	0.483E+01	0.158E+02	0.459E+02	0.329E+02	0.143E+02	0.426E+01	0.880E-01	0.479E-02	0.863E-04
24	56	55	54	53	52	51	50	49	48	47	46
	0.122E-02	0.255E-01	0.349E+00	0.220E+01	0.900E+01	0.166E+02	0.234E+02	0.106E+02	0.187E+01	0.806E-01	0.162E-02
23	55	54	53	52	51	50	49	48	47	46	45
	0.446E-04	0.102E-02	0.143E-01	0.172E+00	0.183E+01	0.511E+01	0.566E+01	0.755E+01	0.405E+01	0.636E+00	0.124E-01
22	54	53	52	51	50	49	48	47	46	45	44
	0.304E-06	0.385E-05	0.219E-03	0.775E-02	0.100E+00	0.413E+00	0.142E+01	0.366E+01	0.330E+01	0.141E+01	0.546E+00
21	53	52	51	50	49	48	47	46	45	44	43
	0.280E-08	0.556E-07	0.546E-05	0.195E-03	0.777E-02	0.577E-01	0.176E+00	0.290E+00	0.621E+00	0.795E+00	0.334E+00
20	52	51	50	49	48	47	46	45	44	43	42
	0.103E-10	0.137E-09	0.191E-07	0.125E-05	0.170E-03	0.182E-02	0.820E-02	0.325E-01	0.108E+00	0.140E+00	0.208E+00

Table IIII. 200 MeV Yield Cross-Section (MB)

YIELD CROSS-SECTION (MB)											
Z\A	60	59	58	57	56	55	54	53	52	51	50
28	0.000E+00	0.614E+01	0.658E+01	0.548E+01	0.153E+01	0.537E-01	0.202E-02	0.596E-04	0.136E-05	0.950E-07	0.610E-09
27	59	58	57	56	55	54	53	52	51	50	49
	0.117E+02	0.257E+02	0.369E+02	0.320E+02	0.163E+02	0.353E+01	0.420E+00	0.204E-01	0.358E-03	0.163E-04	0.727E-07
26	58	57	56	55	54	53	52	51	50	49	48
	0.112E+02	0.112E+02	0.218E+02	0.318E+02	0.519E+02	0.273E+02	0.538E+01	0.191E+00	0.840E-02	0.432E-03	0.338E-05
25	57	56	55	54	53	52	51	50	49	48	47
	0.901E-01	0.719E+00	0.421E+01	0.135E+02	0.423E+02	0.374E+02	0.132E+02	0.421E+01	0.114E+00	0.531E-02	0.125E-03
24	56	55	54	53	52	51	50	49	48	47	46
	0.953E-03	0.211E-01	0.304E+00	0.213E+01	0.996E+01	0.145E+02	0.243E+02	0.157E+02	0.190E+01	0.106E+00	0.531E-02
23	55	54	53	52	51	50	49	48	47	46	45
	0.464E-04	0.986E-03	0.171E-01	0.178E+00	0.166E+01	0.569E+01	0.789E+01	0.907E+01	0.482E+01	0.130E+01	0.263E-01
22	54	53	52	51	50	49	48	47	46	45	44
	0.454E-06	0.662E-05	0.184E-03	0.710E-02	0.140E+00	0.552E+00	0.195E+01	0.326E+01	0.569E+01	0.262E+01	0.652E+00
21	53	52	51	50	49	48	47	46	45	44	43
	0.193E-08	0.563E-07	0.726E-05	0.269E-03	0.763E-02	0.552E-01	0.231E+00	0.479E+00	0.847E+00	0.115E+01	0.755E+00
20	52	51	50	49	48	47	46	45	44	43	42
	0.108E-10	0.223E-09	0.205E-07	0.132E-05	0.190E-03	0.264E-02	0.133E-01	0.394E-01	0.151E+00	0.310E+00	0.447E+00

Table IV. ALICE Parameter Variation for Benchmark 2

Case	MP	INVER	M3	Notes
A	3	2	3	Reference case, pairing correction zero for odd-even nuclei
B	2	2	3	Pairing terms are level density ground state shifted, i.e. include shell corrections so as to refer excitations to liquid drop mass surface
C	3	2	4	Deutrons also emitted
D	3	0	3	Full optical model calculation of inverse cross-sections
E	1	2	3	Like MP=3, but using a backshifted convention with zero shift for even-even nuclei

III.2 Neutron Emission Double Differential Cross-Sections

The benchmark specifications called for results binned in certain secondary angular and energy increments. The results received did not necessarily conform to the specifications. This made tabular comparisons difficult but the results were sufficiently detailed to provide meaningful graphical comparisons.

Data for all three targets AL-27, Co-59, and PB-208 were received from submitters. Additional details are given in Table V.

For ALICE results, the point symbols are plotted at the center of each bin. For HETC-F results, the integrals between energy points on a nonequidistant energy mesh were given and the point symbols are plotted at the arithmetic midpoint of the bins. For HETC-H results, cross-section point symbols are plotted on the energy mesh given, which is assumed to be the bin midpoints. **For improved readability, histogram curves were not drawn through these data.**

The PNEM results were generated on a comparatively fine mesh with a curve connecting the points without symbols.

As an example of the changes that occurred from the draft report, Figure 4 shows the calculated 800 MeV proton induced neutron emission spectrum at 30° . The HETC-H results with corrected normalization are higher by factors of 1 to 3 than the draft report.

A log-linear plot of the per unit lethargy cross-section as shown in Figure 5 is useful for displaying details in neutron emission spectra throughout the energy range. However, the log-log display used in this section is sufficient to globally and compactly compare how well the codes agree without requiring a separate figure for each target and input energy or numerous changes in scale.

While emission spectra can be compared at 10 angles, only selected graphical comparisons will be given. The information has been saved and additional tabular and graphical comparisons can be given at a later time if warranted.

Neutron emission spectra at 15, 30, 60, 90, 120, and 150 degrees are shown in Figures 6, 7, 8, 9, and 10 for 35, 80, 160, 318, and 800 MeV, respectively. The ALICE results at 35, 80, and 160 MeV are the computation format results from ALICE-B obtained with the same input parameters selected by M. Blann. The results have been compared with those of ALICE and are equivalent, except for the small differences indicated earlier. While ALICE-B results for 318 and 800 MeV have been submitted by S. Pearlstein it does not imply that the authors of ALICE, from which ALICE-B was derived, have suggested the use of its algorithms beyond 300 MeV.

Table V. Mesh Sizes of Contributed Benchmarks

<u>Code</u>	<u>Energy</u>	<u>Angle Bin (Deg), Mesh Pts.</u>	<u>Energy Bin (MeV), Mesh Pts.</u>
ALICE ¹	35	5, 36	1, 5
	80	5, 36	1, 7
	160	5, 36	1, 14
ALICE-B ²	318	5, 36	5, 64
	800	5, 36	5, 160
HETC-F ³	35	3-10, 10	2, 12-16
	80	3-10, 10	5, 12-16
	160	3-10, 10	15.5, 11-13
	318	3-10, 10	2.6-118, 11-17
	800	3-10, 10	3.3-328, 11-17
HETC-H ⁴	160	5, 36	10, 16
	318	3, 60	20, 17
	800	3, 60	50, 16
PNEM	All	Continuous	Continuous, 19/decade

NOTES

1. Other ALICE parameters are NA=9, NZ=5, MP=1, INVER=2, M3=0, and I3D=0 (3 dimensional folding). For computerized output, ALICE-B results were used with these parameters.

2. In ALICE-B, ALICE algorithms are extended to 1000 MeV, P values to 70 and the number of secondary energy bins increased for double differential distributions.

3. Results were received at emission angles of 3, 15, 30, 45, 60, 75, 90, 105, 120, 150 degrees. The low energy cut off is 5 MeV.

4. The number of energy bins and bin sizes received differ somewhat from those stated in Appendix II.5.

The angular integrated results and the angular and energy integrated totals, the (p,xn) cross-section, are also of interest. The angular integrated results are shown in Figure 11. The energy-angle integrated totals are listed in Table VI. Figures 6 through 11 can serve as a shape comparisons and Table VI as a magnitude comparison for others calculating these benchmarks.

III.3 Calculation Times

Some information on calculation times was received. From M. Blann's ALICE output from the CDC-7600, a 3.3 MIPS computer, the CPU times for Benchmarks 1 and 2, 1.6 minutes, and at 35, 80, and 160 MeV, for Benchmarks 4 and 5, 2.8 minutes.

PNEM calculation times on the DEC-10, a 0.3 MIPS computer, were 0.8 minutes for each of the Benchmarks 3, 4, or 5.

For the HETC-H calculations received at 160, 318, and 800 MeV for Benchmarks 3, 4, and 5, the timing information is shown in Table VII. The calculations were run on an IBM 3081, a 2.2 MIPS computer. The average benchmark time was 6.5 hours.

Table VI. The (p,xn) Cross-Sections (mb)

Target	Energy	PNEM	ALICE	HETC-F*	HETC-H	Unweighted	
						Av.	Unc.
Al	35	260	460	240		360	100
	80	450	600	350		530	75
	160	710	600	390	660	660	32
	318	1100	990	460	530	870	180
	800	1800	1500	1000	590	1300	360
Zr	35	1200	2200	440		1700	500
	80	2200	2800	730		2500	300
	160	3400	3100	1100	3000	3200	120
	318	5200	4200	1600	1900	3800	980
	800	8800	5400	3600	1500	5200	2100
Pb	35	2800	6100	930		4500	1700
	80	4800	10000	1500		7400	3600
	160	7300	11000	2300	9800	9400	1100
	318	14000	12000	3700	4700	10000	2800
	800	25000	15000	8700	2800	14000	6400

*The energy bins do not extend down to zero energy. This column was not used in the unweighted averages.

Table VII. HETC-H Run Characteristics

<u>Proton Energy (MeV)</u>	<u>Target Material</u>	<u>Number of Source Particles</u>	<u>Run Time On IBM 3081 (h)</u>
800	Pb-208	240000	6.1
316	Pb-208	280000	6.9
160	Pb-208	520000	6.4
800	Zr-90	415000	6.7
316	Zr-90	640000	5.3
160	Zr-90	1040000	8.6
800	Al-27	1080000	5.3
316	Al-27	1580000	5.3
160	Al-27	2650000	7.5

IV. Discussion

IV.1 Activation Yields

The results from ALICE and ALICE-B were identical except where λ values greater than 21 were invoked. The main purpose of the calculations presented here were to show the effect of ALICE options on the results.

The calculated results of 180 MeV protons on Al-27 shown in Fig. 2 are not compared with experiment here but follow the physical form expected. Each activated element has an isotopic distribution that peaks at a mass value appropriate to the energetics of the reactions. The peak mass value for each element decreases about one unit for each unit of decreasing charge.

Figure 2 shows that the cross-sections for activating low Z elements from a Co-59 target increases with input proton energy as more energy is available.

In Figure 3 the yield cross-sections for activation products can be seen to vary up to approximately a factor of 2 depending on the model parameters chosen. The inclusion of deuteron emission as in Case C and use of a backshifted pairing term without shell corrections as in Case E produce about the same results as the reference Case A. The use of the backshifted pairing terms with shell corrections as in Case B and the optical model calculation of the inverse reaction cross-section as in Case D lowers the activation cross-section of Co-56 and raises the activation cross-sections of Mn-54 and V-50 compared to the reference Case A.

IV.2 Neutron Emission Double Differential Cross-Sections

Detailed differences among the calculations submitted can be observed by examining Figures 6 through 10. Some overall conclusions will be attempted here. In general, the calculated emitted neutron energy distribution shows a quasielastic peak, i.e., the apparent elastic scattering of the incident proton with a target neutron, in the forward angles. For small scattering angles the peak is sharp and near the incident proton energy. As the emission angle increases the peak is broadened and occurs at a lower energy as expected from the kinetics of elastic reactions.

The two sets of HETC calculations submitted can be compared at 160, 318, and 800 MeV. The calculated shapes are similar and the corrected normalization HETC-H calculations and the HETC-F calculations are in general agreement.

At back angles PNEM calculates more high energy neutrons than calculated by the other codes.

There is good overall agreement in magnitude among the codes at forward angles. Differences, where they occur, at the forward angles, are greatest for mid energy neutrons.

The differences that occur in the double differential angular and energy distributions are primarily due to differences among the code models. PNEM, because of its empirically determined parameters, calculates a greater high energy neutron emission at back angles than the other codes. At high incident energies the back angle high energy neutron emission from HETC calculations is greater than that from ALICE-B. The HETC modeling includes more particle-particle kinetics than the ALICE modeling. The development of HETC has been primarily based on physics data above 100 MeV whereas the development of ALICE has been primarily based on physics data below 100 MeV. Although the HETC model calculations are expected to be valid only above 150 MeV where the nucleon de Broglie wave length is lower than the mean free path in the nucleus, at least for these benchmarks, there are no large differences between the ALICE and HETC-F results at 35 and 80 MeV.

The angular integrated energy distributions of Fig. 11 show closer agreement among the methods than shown in individual double differential views. The methods agree in magnitude except for A1 at 35 and 80 MeV where the PNEM extrapolation of high energy systematics to low energy lies below the other calculations. At high energies the preequilibrium and evaporation components of the ALICE-B calculations are clearly visible.

The integrated total (p,xn) cross-sections are mostly determined by the nearly isotropic low energy neutron evaporation spectrum that peaks about 1 MeV and are not strongly influenced by the major differences among the methods that occur at back angles where the cross-sections are small. The percentage unweighted uncertainty in Table VI is less than 30% except for Zr at 800 MeV and Pb at 35, 80, and 800 MeV. The energy at which the best overall agreement is obtained is 160 MeV and the material for which best overall agreement is obtained is Al.

IV.3 Calculation Times

Correcting for the speed differences among the computers used, the running times among the calculational methods submitted can be approximately compared. Each of the Benchmarks 3, 4, or 5 can be calculated by PNEM in the order of seconds, ALICE or ALICE-B in the order of minutes and HETC-F or HETC-H in the order of tens or hundreds of minutes.

V. Summary

The study illustrated the results of using a preequilibrium plus evaporation model code to calculate the activation of materials by proton bombardment and the results of three types of model codes to calculate proton induced double differential neutron emission spectra. Circulation of the draft report was useful to obtain refinements and corrections that could be included in the benchmark comparison. For double-differential data, there was generally good agreement among the codes at forward angles. At back angles, the calculated neutron emission varied widely among the codes with results from nuclear systematics significantly above the others. The global graphical presentation of the results for double differential data together with timing data about typical computer runs gives the reader information that can be used to determine cost effective methods for his applications.

VI. Acknowledgments

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References

1. S. Pearlstein, Summary of the Meeting of the Medium Energy Nuclear Data Working Group, May 27-29, 1987. BNL-NCS-40070, Informal Report.
2. M. Blann, Phys. Rev. C28, 1475 (1983).
3. H. W. Bertini, Phys. Rev. 188, 1711 (1969).
4. S. Pearlstein, Nucl. Sci. and Eng. 95, 116 (1987).

APPENDIX I

Proposed MENDWG Benchmark Problem

Activation Yields

180 MeV $p + {}^{27}\text{Al}$

40 MeV + 200 MeV $p + {}^{59}\text{Co}$ (all yields)

E_p step = 10 MeV, i.e., $E_p = 40, 50, 60, \dots, 200$

Double Differential Cross-section for Neutron Emission

$d^2\sigma/d\epsilon d\Omega$ (p,xn) inclusive

Targets ${}^{27}\text{Al}$, ${}^{90}\text{Zr}$, ${}^{208}\text{Pb}$

$E_p = 35$ MeV - θ step = 5° , $d\theta$ bin = 5° , θ center = 2.5° ,
i.e., $\theta = 2.5^\circ, 7.5^\circ, 12.5^\circ, \dots$;
 E' step = 5 MeV, dE' bin = 1 MeV, E' center = 5 MeV,
i.e., $E' = 5, 10, 15, \dots$ MeV.

$E_p = 80, 160$ MeV - θ step = 5° , $d\theta$ bin = 5° , θ center = 2.5° ,
i.e., $\theta = 2.5^\circ, 7.5^\circ, 12.5^\circ, \dots$;
 E' step = 10 MeV, dE' bin = 1 MeV, E' center = 5 MeV,
i.e., $E' = 5, 15, 25, \dots$ MeV.

$E_p = 318$ MeV - θ step = 3° if possible, $d\theta$ bin = 3° , θ center = 1.5°
i.e., $\theta = 1.5^\circ, 4.5^\circ, 7.5^\circ, \dots$;
 E' step = 20 MeV, dE' bin = 1 MeV, E' center = 5 MeV
i.e., $E' = 5, 25, 45, \dots$ MeV.

$E_p = 800$ MeV - θ step = 3° if possible, $d\theta$ bin = 3° , θ center = 1.5°
i.e., $\theta = 1.5^\circ, 4.5^\circ, 7.5^\circ, \dots$;
 E' step = 50 MeV, $dE' = 1$ MeV, E' center = 50 MeV
i.e., $E' = 50, 100, 150, \dots$ MeV.

Results are to be sent to S. Pearlstein, National Nuclear Data Center, Building 197D, Upton, NY 11973, with a description or reference of the code, input parameters, and other relevant factors. The output must be in tabular form to facilitate comparison with other calculations. To be included in this comparison results should be received by 1 November 1987.

Appendix II - Code Abstracts

II.1 PNEM

1. Identification - PNEM - High energy double differential neutron emission and other proton and neutron induced cross-sections.
2. Computer for which software is written and other machine versions available. - DEC 10
3. Description - For high energy incident protons and neutrons, the code calculates double differential neutron emission, differential nuclear elastic, total (for neutrons) and scattering cross-sections. Angular integrated, energy integrated, and angular and integrated neutron emission cross-sections are optionally calculated.
4. Method of Solution - Parametric fits to the systematics of nuclear data.
5. Status - Preliminary version PNEM1 first available in November 1985. Second version PNEM2 available in July 1986, revised in September 1987. PNEM2 is being field tested by a few collaborators and has not been distributed for general use.
6. Restrictions - Nuclear mass range 6 to 265.
7. References -

Primary reference -
S. Pearlstein, Nucl. Sci. Eng. 95, 116-127 (1987).

Secondary references -
J. Letaw, et. al., Astrophys. J. Supp. Series 51, 271-276 (1983).
Angeli and J. Csikai, Nucl. Phys. A170, 577-583 (1971).
S. Pearlstein, Nucl. Sci. Eng. 49, 162-171 (1972).
8. Hardware Requirements - Ordinary.
9. Programming Language - FORTRAN 77.
10. Operating System requirements - Ordinary.
11. Name and establishment of author or submitter -
Sol Pearlstein
National Nuclear Data Center
Brookhaven National Laboratory
Upton, New York 11973
(516) 282-2901, FTS 666-2901
12. Material Available - See Status.

II.2 ALICE

1. Identification - ALICE/LIVERMORE 85/300 precompound compound decay.
2. Computer for which Software is Written and Other Machine Versions Available - CDC 6700 (designed to be machine-dependent).
3. Description - ALICE/LIVERMORE 85 calculates particle spectra and yields for precompound plus compound decay, including fission competition. Multiple decay of neutron (n), proton (p), alpha, and deuteron (d) particles may be considered. The program can perform a standard Weisskopf-Ewing evaporation calculation with multiple particle emission or an s-wave approximation calculation which gives an upper limit to the enhancement of gamma ray de-excitation due to angular momentum effects. The evaporation calculation can include fission competition according to the Bohr-Wheeler approach, using angular momentum dependent ground state and saddle point energies. (The latter values are derived from Cohen, et al, rotating liquid drop model or Sierks finite range model.) Provision to permit precompound emission via the hybrid and geometry-dependent hybrid models is included.
4. Method of Solution - In the Weisskopf evaporation calculation, the inverse reaction cross sections may be provided as input data or computed with a classical sharp cutoff algorithm or an optical model routine. In the s-wave approximation the calculation is performed for every partial wave in the entrance channel. The transmission coefficients for the entrance channel partial waves may be provided as input data or by the parabolic model or optical model calculation. The Myers-Swiatecki/Lysekil mass formula is used to calculate the Q value for formation of the compound nucleus and the n, p, alpha, and d binding energies for all nuclides of interest in the evaporation chain, or experimental masses (available in a library subroutine) can be used.
5. Restrictions on the Complexity of the Problem - Excitation energies of the compound nucleus up to 200 MeV can be considered in the Weisskopf evaporation calculation. In the s-wave approximation it is assumed that the rotational energy for each partial wave is irrevocably committed to rotational motion and, therefore, unavailable for particle emission.
6. Timing - The sample problem execution time is approximately 10 seconds on a CDC 7600 and 40 seconds on an IBM 3033.
7. Unusual Features of the Software - None, standard FORTRAN IV.
8. Related and Auxiliary Software - ALICE/LIVERMORE 85 is a revision of the earlier ALICE and OVERLAID ALICE codes.

9. Status - Abstract first distributed April 1984.
CDC 7600 version submitted November 1983, sample problem executed by NESC December 1983 on an IBM 3033.
10. References - M. Blann and J. Bisplinghoff, CODE ALICE/LIVERMORE 82, UCID-19614 November 5, 1982; M. Blann, CODE ALICE/85/300, UCID 20169 (October 1984).
ALICE/LIVERMORE 82, NESC No. 1036, ALICE/LIVERMORE 82 Tape Description and Implementation Information, National Energy Software Center Note 84-28, April 30, 1984.
M. Blann, OVERLAID ALICE: A Statistical Model Computer Code including Fission and Preequilibrium Models, COO-3494-29, August 1976.
11. Hardware Requirements - NESC used approximately 244K bytes on an IBM 3033 to execute the sample problem.
12. Programming Language - FORTRAN IV.
13. Operating System - SCOPE (CDC 7600), OS/MVT (IBM 3033).
14. Other Programming or Operating Information or Restrictions - The FORMAT statements contain " delimiters.
15. Name and Establishment of Author or Contributor -
M. Blann
Lawrence Livermore National Laboratory
J. Bisplinghoff
Institut fuer Strahlen und Kernphysik
Bonn University
Germany
16. Material Available
Source
Sample problem input
Sample problem output
Reference report, UCID 20169
17. Keywords - evaporation model, compound nucleus reactions, precompound-nucleus emission, Weisskopf model, Bohr-Wheeler theory, nuclear models.
18. Sponsor - DOE Office of High Energy and Nuclear Physics.

II.3 ALICE-B

1. Identification - ALICE-B
2. Computer for which Software is Written - DEC-10, VAX-780
3. Description - Derived from ALICE/LIVERMORE 85. Its algorithms extended to 1000 MeV. The user should be warned that the physics may not be applicable at these energies. Partial wave analysis extended to $l=70$. Number of energy bins for angular distributions increased. Above 300 MeV the optical model cross-section is corrected.
4. Unusual Features of the Software - G-Floating point arithmetic.
5. Related and Auxiliary Software - ALICE-B is an informal revision of ALICE/LIVERMORE 85.
6. Status - Experimental. All changes communicated to M. Blann, author of ALICE/LIVERMORE 85/300 for possible inclusion in future versions.
7. References - S. Pearlstein, private communication.
8. Programming Language - FORTRAN IV.
9. Name and Establishment of Author or Contributor -
S. Pearlstein
Building 197D
Brookhaven National Laboratory
Upton, NY 11973
10. Material Available - None.
11. Keywords - evaporation model, compound-nucleus reactions, precompound-nucleus emission, Weisskopf model, Bohr-Wheeler theory, nuclear models.

II.4 HETC-CCC-178

Since HETC-F and HETC-H make extensive use of RSIC Code Package -178, information on RSIC Code Package CCC-178 is included.

1. Identification - HETC: Monte Carlo High Energy Nucleon Meson Transport Code System.

Auxiliary Routines -

COPY: Utility routine
PUNCROSS: Cross Section Handling Code
HET: Nucleon-Meson Transport Code
NMTA: Data Processing Code
EHET: Edit Code
XSECT: Cross Section Data Generator
O5R: Modified Monte Carlo Code (CCC-17).
O5RA: O5R Sample Problem Analysis Code
HETC is basically an extension of CCC-161/NMTC.

2. Contributor - Oak Ridge National Laboratory, Oak Ridge, Tennessee.
3. Coding Language and Computer - FORTRAN IV; IBM 360/370.
4. Nature of Problem Solved - HETC is a Monte Carlo transport code for computing the properties of high-energy nucleon-meson cascades in matter. It is basically an extension of CCC-161/NMTC (valid for energies < 3 GeV) to allow particle transport up to several hundred GeV.

The source particle description is specified in a user-written subroutine and may be arbitrarily distributed in energy, direction, and space. Proton, neutron, π^+ , π^- , μ^+ , and μ^- sources are allowed.

Although the maximum allowable source particle energies are not well defined, HETC has been run successfully for energies up to 1 TeV. However, because of the lack of experimental data at very high energies, comparison of HETC results with experimental data have been made only for energies < 30 GeV.

The code stores on magnetic tape a complete description of each "event" (nuclear interaction, geometry boundary crossing, pion decay, etc.) that occurs during the transport process. This information is then read and processed by user-written analysis programs to obtain results for a particular problem.

Differential cross sections for nucleon-nucleus and pion-nucleus nonelastic collisions are not required as input since they are, in effect, computed in the course of the transport calculation using the intranuclear-cascade-extrapolation-evaporation model.

Since HET provides a complete description of the low energy (< 15 MeV) neutron production, HET may be readily coupled with codes other than 05R (e.g., CCC-254/ANISN, CCC-209/DOT, CCC-203/MORSE) to obtain the low energy neutron transport.

5. Method of Solution - HETC consists of two basic transport codes: HET and a modified version of 05R. HET transport particles in the energy range from the source-particle energy down to a specified energy cutoff, which is commonly taken to be 15 MeV for protons and neutrons, 2 MeV for charged pions, and 0.2 MeV for muons. Neutrons produced in HET below the cutoff energy are transported via the 05R code.

The description of nonelastic-collision products in HET is obtained using an intranuclear-cascade-extrapolation-evaporation model. At each nonelastic collision a calculation is performed using subprogram versions of Bertini and Guthrie's latest intranuclear-cascade program (Nucl. Phys. A169, 670 (1971)) and Guthrie's evaporation program (ORNL-TM-3119) to determine the energy and direction of emitted cascade nucleons and pions and evaporated nucleons, deuterons, tritons, (ORNL-TM-3667) He-3's, and alpha particles and the mass, charge the recoil energy of the residual nucleus. For nonelastic collisions < 3 GeV, these intranuclear-cascade-evaporation results are used directly; for nonelastic collisions > 3 GeV, the results from an intranuclear-cascade-evaporation calculation at approximately 3 GeV are scaled to the proper energy using the extrapolation method of Gabriel, Alsmiller, Jr., and Guthrie. Nonelastic collisions with hydrogen nuclei are treated using experimental data and the calculation method of Gabriel, Santoro, and Barish (ORNL-TM-3615). Nonelastic collisions in 05R are treated using the evaporation model in conjunction with experimental cross sections. Experimental data are used for elastic-collision cross sections.

Charged-pion and muon decay in flight and at rest are taken into account using known lifetimes.

6. Restrictions or Limitations - Present dimensions restrict the number of different media to 15 or less and the number of types of nuclei per medium to 11 or less. Virtually arbitrary geometries may be specified.
7. Typical Running Time - Running time is extremely problem dependent. A sample problem included with the code documentation required approximately 10 minutes on the IBM 360/91 and approximately 3 times longer on the IBM 360/75.
8. Computer Hardware Requirements - HETC is operable on the IBM 360/370 computers. Approximately 1000K bytes of memory and 4 peripheral storage devices are required.

9. Computer Software Requirements - A FORTRAN H compiler is required.

10. References

K. C. Chandler and T. W. Armstrong, "Operating Instructions for the High-Energy Nucleon-Meson Transport Code HETC," ORNL-4744 (January 1972).

W. A. Coleman and T. W. Armstrong, "The Nucleon-Meson Transport Code NMTC," ORNL-4606 (October 1970).

T. W. Armstrong and K. C. Chandler, "NMTA--Analysis Subroutines for the Nucleon-Meson Transport Code NMTC," ORNL-4736 (November 1971).

D. C. Irving, R. M. Freestone, Jr., and F. B. K. Kam, "O5R, A General-Purpose Monte Carlo Transport Code," ORNL-3622 (February 1965).

D. C. Irving, W. E. Kinney, and Pat Rea, "LEGENDRE, A Program to Calculate Legendre Coefficients from Angular Distributions," ORNL-TM-1241 (November 1965).

D. C. Irving, V. R. Cain, and R. M. Freestone, "An Amplification of Selected Portions of the O5R Monte Carlo Code User's Manual," ORNL-TM-2601 (May 1969).

T. W. Armstrong, R. G. Alsmiller, Jr., K. C. Chandler, and B. L. Bishop, "Monte Carlo Calculation of High-Energy Nucleon-Meson Cascades and Comparison with Experiment," ORNL-TM-3667 (January 1972).

James B. Langworthy, "An Organizational Description of High Energy Transport Code (HETC)," NRL Memorandum Report 2729 (June 1974).

11. Contents of Code Package - Included are the referenced documents and a reel of magnetic tape which contains source decks, random number generators, input data written in BCD/EBCDIC card images, plus output written in list format; total records 62,533 (A) and 5486 (B).

12. Date of Abstract - December 1974; updated May 1975.

13. Keywords - Monte Carlo, nucleon; neutron; proton; meson; complex geometry; high energy.

14. Availability - Contact Radiation Shielding Information Center, Oak Ridge National Laboratory, P.O. Box X, Oak Ridge, TN 37831-6362, Telephone (615) 574-6176.

II.5 HETC-H Description and Computational Details

KFA-Version of HETC and Description of the Procedure to Calculate Cross-Sections

HETC-KFA-2 in the HERMES System

To simulate the histories, i.e. production, interaction with matter and transport, of high energetic particles the latest state-of-the-art radiation transport codes and event generators are used in HERMES. All used codes employ Monte Carlo techniques with 3 dimensional geometry description, therefore, it is possible to treat in detail the reaction mechanism and the transport of the high energy particles as well as of the low-energy particles created. An overview of the main physics models is given in Ref. 1. Some details about the hadron cascade module HETC-KFA-2 used at KFA are given below.

HETC (High Energy Transport Code) is implemented in a version based on the original coding given in Ref. 2. Other important references about the models are given in Refs. 3 and 4.

Name:	HETC-KFA-2	(High-Energy-Radiation-Transport-Code, KFA Version 2)
Implementation:	based on Ref. 2 (Report ORNL-4744)	
Extension:	FORTRAN77 compatible on IBM3081 and CRAY-XMP22	
Particles transported:	n, p, $\pi^{\pm}$, $\mu^{\pm}$	
Extension:	d, t, He^3 , α , heavy ions $A < 20$	
Mechanism:	- collision model - Intranuclear-Cascade-Evaporation (INCE) (for p,n,$\pi^{\pm}$; π^- capture at rest; non-elastic nuclear collisions, nonelastic hydrogen collisions; π^0,d,t,He^3,α-production; residual nuclei and residual excitation energy) - charged particle ionization energy loss (dE/dx) - primary particle small angle multiple Coulomb scattering - decay (weighted fashion) for $\pi^{\pm}$ and $\mu^{\pm}$ in flight and at rest	

- scaling model - automatic parameter update for nonelastic collisions above 3.5 GeV
(limited energy range for scaling
pn - $E_{\max} \leq 25$ GeV
 $\pi^{\pm}$ - $E_{\max} \leq 15$ GeV)

Extensions:

- elastic collision module for p/n elastic nucleus collisions upto 20 GeV
- high energy fission included in evaporation model
- automatic parameter update for B_0 in level density formula
- nonisotropic angular distribution of evaporated particle
- analog decay for $\pi^{\pm}$

Geometry: standard CG geometry interface

Extension: CG-KFA geometry module

Additional submission of particles and nuclei for

Extensions: further processing structure of HERMES structure of HERMES submission files

The cross-section calculations were performed with the HETC-KFA-2 for the present benchmark with a so called thin target setup. This means that only the intranuclear cascade evaporation model is used. The emitted neutrons in this model are not able to undergo further nuclear reactions with other nuclei. For all targets the variable B_0 -option of the code and a isotropic emission for evaporation was assumed while high energy fission was excluded. All cases were run with about 5 to 7 hours computer time on IBM-3081. The number of incident protons (Table 3) and also the binning of the energy intervals were chosen in a way that even at energies and angles with a low probability for neutron emission an acceptable neutron yield could be determined. This means, that in the average at every energy-angle-bin at least more than 100 emitted neutrons were sampled.

In the current version of HETC-KFA-2 neutron production spectra are determined by defining yield detectors for the analysis of the specific nuclear reaction. A detector has to be understood as an analysis about some criteria for example the type, energy and emission angle of particles (Table 1). Therefore, the HETC output contains the neutron yield in predefined energy and angle ranges normalized to the number of source protons and referred to a nuclear density of unity. The double differential cross-section is then calculated by the following procedure.

$$d^2\sigma/dE d\Omega \text{ [b/(MeV} \cdot \text{sr)]} = Y_{\text{HETC}} \cdot \Sigma_G \cdot 1/\Delta E_i \cdot 1/(2\pi \sin\theta_j \cdot \Delta\theta_j)$$

with

Y_{HETC} neutron yield, normalized to 1 incident proton and a nuclear density of 1.
 Σ_G geometric cross-section
 ΔE $E_{i+1}-E_i$
 E_i, E_{i+1} group boundaries of energy interval i
 $\Delta\theta_j$ $\theta_{j+1} - \theta_j$
 θ_j, θ_{j+1} interval boundaries of angle interval

The transparency factor in the HETC-KFA-2 has not to be considered any more like in former versions. The values of geometric cross-sections are given in Table 2.

Energy [MeV] [MeV]	No. of Energy-bins	Width of Energy-bins [MeV]	No. of Angle-bins	Width of angle-bins [degree]
160.	16.	10.	36.	5.0
318.	31.	10.	60.	3.0
800.	40.	20.	60.	3.0

Table 1: Energy- and angle binning used for MENDWG benchmark problem

Target Nucleus	Proton- Energy [MeV]	Geometric Cross Section [barn]	Transparency of the Nucleus
Al-27	160	1.0282	0.400
	318	1.0282	0.386
	800	1.0282	0.476
Zr-90	160	1.6769	0.560
	318	1.6769	0.548
	800	1.6769	0.623
Pb-208	160	2.4615	0.662
	318	2.4615	0.647
	800	2.4615	0.706

Table 2: Geometric cross sections and transparencies of the nuclei Al-27, Zr-90 and Pb-208 at the thin-target calculations with HETC/KFA-2

Proton Energy [MeV]	Target Nuclide	Number of Source Protons	Number of real collisions	Run time on IBM 3081 [h]
800	Pb-208	240000	169400	6.1
316	Pb-208	280000	181200	6.9
160	Pb-208	520000	344200	6.4
800	Zr-90	415000	258500	6.7
316	Zr-90	640000	247000	5.3
160	Zr-90	1040000	582400	8.6
800	Al-27	1080000	514100	5.3
316	Al-27	1580000	609900	5.3
160	Al-27	2650000	1060000	7.5

Table 3: Statistic of the computational procedures of cross-section calculations for the NENDWG benchmark problems with HETC/KFA-2

References

- /1/ P. Cloth, D. Filges, R.D. Neef, G. Sterzenbach, Ch. Reul,
T.W. Armstrong, B.L. Colborn, B. Anders, H. Brückmann
HERMES - High Energy Radiation Monte Carlo Elaborate
System
KFA Jül-Report, in preparation

- /2/ T.W. Armstrong, K.C. Chandler
HETC, Monte-Carlo High Energy Nucleon Meson Transport Code
ORNL-4744, January 1972

- /3/ T.W. Armstrong, K.C. Chandler
HETC - A High Energy Transport Code
Nucl.Sci. and Eng. 49, 110 (1972)

- /4/ Monte Carlo High-Energy Nucleon-Meson Transport Code
Oak Ridge National Laboratory
RSIC Computer Code Collection, CCC-178

II.6 HETC-F (TIERCE)

I NAME AND TITLE

TIERCE : (Transport des Ions et des Radiations dans les Cibles
Epaisses)

Auxillary Routines :

HETC : Nucleon-Meson Transport Code (CCC-178/HETC)

EHET : Edit Code

MORSE : Modified Monte Carlo Code (CCC-203/Morse C.G)

Tierce is an extensive modification of CCC-178/HETC.

II CODING LANGUAGE AND COMPUTER

FORTRAN 77 ; IBM 3090/200

III NATURE OF PROBLEM SOLVED

Tierce is a Monte-Carlo transport code system for computing the properties of high-energy nucleon meson cascades in matter. It is basically an extension of CCC-178/HETC (valid for energies up to several hundred GeV).

The source particle description is specified in a user-written subroutine and may be arbitrarily distributed in energy, direction, and space. Proton neutron, Pi^+ , Pi^- , μ^+ , μ^- , and light ion ($A \leq 8$) sources are allowed.

For the target description the combinatorial geometry is used.

Each event (nuclear interaction, geometry boundary crossing, pion decay, etc...) that occurs during the transport process is analysed "on-line", according to the user choice. However, an history tape can be generated if necessary, to be read and processed "off-line" to obtain results for a particular problem.

Differential cross sections for nucleon-nucleus and pion-nucleus, nonelastic collisions are not required as input since they are in effect, computed in the course of the transport calculation using the intranuclear-cascade-evaporation model.

The low energy neutron (≤ 15 MeV) transport is processed by MORSE which is coupled with HETC.

The results obtained by the different modules can be merged and synthesized under graphic representation according to user choice.

IV - METHOD OF SOLUTION

TIERCE consists of two basic transport codes : HETC and a modified version of MORSE. HETC transport particles in the energy range from the source-particle energy down to a specified energy cutoff, which is commonly taken to be 15 MeV for protons and neutrons, 2 MeV for charged pions, and 1.6 MeV for muons. Neutrons produced in HETC below the cutoff energy are transported via the MORSE code.

The description of nonelastic-collision products in HETC is obtained using an intranuclear-cascade-extrapolation-evaporation (with fission). For $A \geq 1$ incident particle, the nucleons giving a non-elastic collision are treated under either evaporation or intranuclear-cascade-evaporation model. In the later case a calculation is performed using subprogram versions of Bertini and Guthrie's latest intranuclear-cascade program (Nucl. Phys. A169, 670 (1971)) and Guthrie's evaporation program (ORNL-TM-3119) to determine the energy and direction of emitted cascade nucleons and pions and evaporated nucleons, deuterons, tritons, (ORNL-TM-3667) He^3 's, and alpha particles and the mass, charge, recoil energy of the residual nucleus. For nonelastic collisions ≤ 3 GeV, these intranuclear-cascade-evaporation results are used directly; for nonelastic collisions ≥ 3 GeV, the results from an intranuclear-cascade-evaporation calculation at approximately 3 GeV are scaled to the proper energy using the extrapolation method of Gabriel, Alsmiller, Jr., and Guthrie. Nonelastic collisions with hydrogen nuclei are treated using experimental data and the calculation method of Gabriel, Santoro, and Barish (ORNL-TM-3615). Nonelastic collisions in MORSE are treated using experimental neutron cross sections. Experimental data are used for elastic-collision cross sections.

Charge-pion and muon decay in flight and at rest are taken into account using known lifetimes.

Fig. 1. Yield Cross-Sections of Activation Products from 180 MeV Protons on Al-27

Fig. 2. Yield Cross-Sections of Activation Products from a) 120, b) 160, and c) 200 MeV Protons on Co-59.

(b)

(c)

Fig. 3. Yield Cross-Sections of Activation Products from Protons on Co-59. See text for explanation of symbols A through E.
a) Co-56, b) Mn-54, c) V-50

Fig. 4. Neutron energy spectra from 160 MeV protons on Al-27, Zr-90 and Pb-208 at an emission angle of 30 degrees 4(a) Draft report, 4(b) Final report.

Fig. 5. Neutron energy spectra from Pb-208. Same data as Figure 4(b) but plotted on a log-linear scale with the cross-section per unit lethargy.

Fig. 6. Neutron energy spectra from 35 MeV protons on Al-27, Zr-90 and Pb-208 at emission angles 15, 30, 45, 60, 90, 120, and 150 degrees.

Fig. 6. cont.

Fig. 7. Neutron energy spectra from 80 MeV protons on Al-27, Zr-90 and Pb-208 at emission angles 15, 30, 45, 60, 90, 120 and 150 degrees.

Fig. 7. cont.

Fig. 8. Neutron emission spectra from 160 MeV protons on Al-27, Zr-90 and Pb-208 at emission angles 15, 30, 45, 60, 90, 120 and 150 degrees.

Fig. 8. cont.

Fig. 9. Neutron energy spectra from 318 MeV protons on Al-27, Zr-90 and Pb-208 at emission angles 15, 30, 45, 60, 90, 120 and 150 degrees.

Fig. 9. cont.

Fig. 10. Neutron energy spectra from 800 MeV protons on Al-27, Zr-90 and Pb-208 at emission angles 15, 30, 45, 60, 90, 120 and 150 degrees.

Fig. 10. cont.

Fig. 11. Angular integrated neutron emission data at 35, 80, 160, 318 and 800 MeV from Al-27, Zr-90 and Pb-208.

Fig. 11. cont.